

=> d his full

(FILE 'HOME' ENTERED AT 15:52:22 ON 11 DEC 2005)

FILE 'CASREACT' ENTERED AT 15:52:35 ON 11 DEC 2005

L1 STRUCTURE UPLOADED

D QUERY

L2 0 SEA SSS SAM L1 (0 REACTIONS)

L3 1 SEA SSS FUL L1 (1 REACTIONS)

D L3

FILE 'CAPLUS' ENTERED AT 15:53:15 ON 11 DEC 2005

L4 1 SEA ABB=ON PLU=ON L3

D L4

FILE 'CASREACT' ENTERED AT 15:53:33 ON 11 DEC 2005

L5 STRUCTURE UPLOADED

D QUERY

L6 0 SEA SSS SAM L5 (0 REACTIONS)

L7 3 SEA SSS FUL L5 (3 REACTIONS)

D L7 1-3

FILE 'CAPLUS' ENTERED AT 15:55:40 ON 11 DEC 2005

L8 3 SEA ABB=ON PLU=ON L7

D L8 1-3 ABS IBIB

FILE HOME

FILE CASREACT

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FILE CONTENT:1840 - 11 Dec 2005 VOL 143 ISS 24

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*
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This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE CAPLUS

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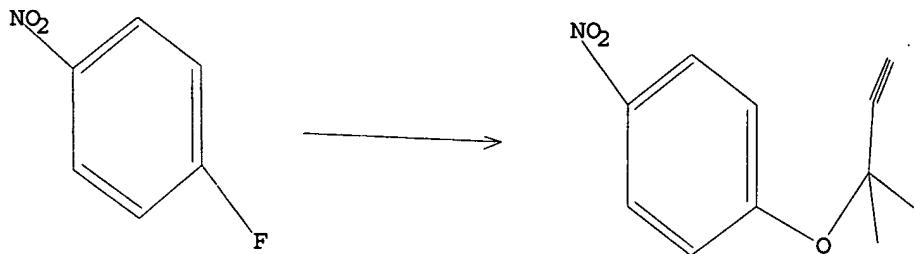
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FILE COVERS 1907 - 11 Dec 2005 VOL 143 ISS 25
FILE LAST UPDATED: 9 Dec 2005 (20051209/ED)

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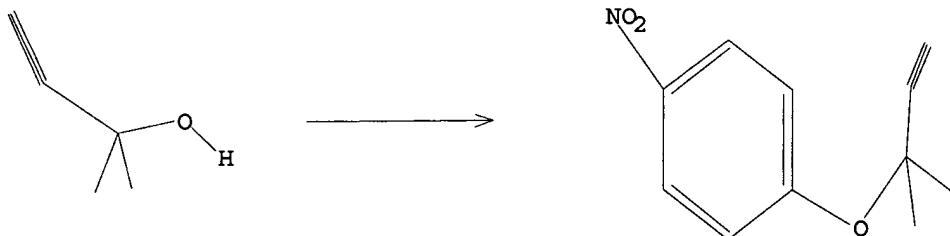
<http://www.cas.org/infopolicy.html>

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L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

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L5 HAS NO ANSWERS
L5 STR



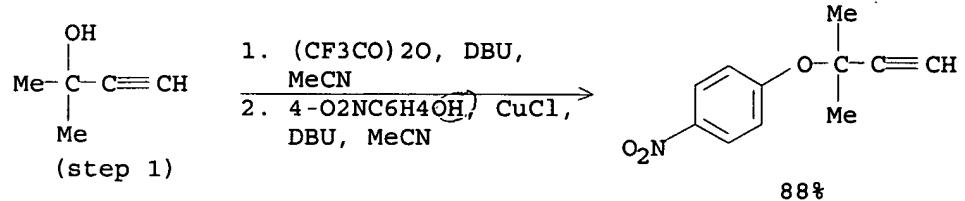
Structure attributes must be viewed using STN Express query preparation.

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
AB An efficient, general, and practical synthesis of aryl
1,1-dimethylpropargyl ethers has been developed. Thus, alkylation of
RC₆H₄OH (R = e.g., 4-CN, 4-NO₂) with HC.tpbond.CCMe₂X (X = Cl, OCO₂Me,
O₂CCF₃) in MeCN containing DBU and Cu salts resulted in high yield of
propargyl ethers RC₆H₄OCMe₂C.tpbond.CH (up to 88%).

ACCESSION NUMBER: 1995:65983 CAPLUS
DOCUMENT NUMBER: 122:9577
TITLE: Improved synthesis of aryl 1,1-dimethylpropargyl
ethers
AUTHOR(S): Godfrey, Jollie D., Jr.; Mueller, Richard H.;
Sedergran, Thomas C.; Soundararajan, Nachimuthu;
Colandrea, Vincent J.
CORPORATE SOURCE: Chem. Process Research, Bristol-Myers Squibb,
Princeton, NJ, 08543-4000, USA
SOURCE: Tetrahedron Letters (1994), 35(35), 6405-8
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 122:9577

RX(4) OF 12

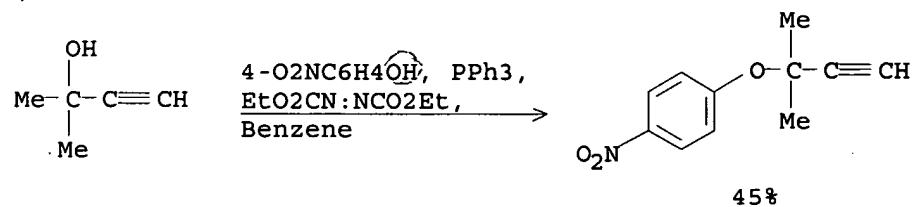


REF: Tetrahedron Letters, 35(35), 6405-8; 1994

L8 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
AB The synthesis of aryl ethers of ethynyl carbinols using the Mitsunobu reaction is reported. Thus, a mixture of HC.tplbond.CCMe2OH and 4-MeC6H4OH in C6H6 was treated with Ph3P and EtO2CN:NCO2Et to give 55% 4-MeC6H4OCMe2.tplbond.CH. Eleven similar examples are also reported.

ACCESSION NUMBER: 1990:178193 CAPLUS
DOCUMENT NUMBER: 112:178193
TITLE: A facile synthesis of aryl ethers of ethynyl-carbinols using the Mitsunobu reaction
AUTHOR(S): Subramanian, R. Sankara; Balasubramanian, K. K.
CORPORATE SOURCE: Dep. Chem., Indian Inst. Technol., Madras, 600 036, India
SOURCE: Synthetic Communications (1989), 19(7-8), 1255-9
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CODEN: SYNCV; ISSN: 0039-7911
OTHER SOURCE(S): CASREACT 112:178193

RX(7) OF 11



REF: Synthetic Communications, 19(7-8), 1255-9; 1989

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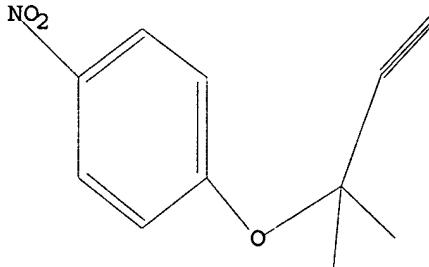
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COST IN U.S. DOLLARS		SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST		0.86	1.07

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Uploading C:\Program Files\Stnexp\Queries\acetylene.str

L2 STRUCTURE UPLOADED

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L2 HAS NO ANSWERS
L2 STR



Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED -          1 TO ITERATE

100.0% PROCESSED      1 ITERATIONS          0 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:      1 TO      80
PROJECTED ANSWERS:         0 TO      0
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1.3 0 SEA SSS SAM 1.3

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FULL SCREEN SEARCH COMPLETED -          21 TO ITERATE
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100.0% PROCESSED 21 ITERATIONS 3 ANSWERS
SEARCH TIME: 00.00.01

For additional information, please consult the following help messages:

HELP DFIELDS -- To see a complete list of individual display fields.
HELP FORMATS -- To see detailed descriptions of the predefined formats.
ENTER DISPLAY FORMAT (IDE):end

=> d his

(FILE 'HOME' ENTERED AT 16:32:16 ON 11 DEC 2005)

FILE 'REGISTRY' ENTERED AT 16:32:39 ON 11 DEC 2005

L1	STRUCTURE UPLOADED
L2	STRUCTURE UPLOADED
L3	0 S L2 SSS SAM
L4	3 S L2 SSS FULL

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	164.34	164.55

FILE 'CAPLUS' ENTERED AT 16:38:28 ON 11 DEC 2005

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FILE COVERS 1907 - 11 Dec 2005 VOL 143 ISS 25
FILE LAST UPDATED: 9 Dec 2005 (20051209/ED)

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<http://www.cas.org/infopolicy.html>

=> s 14
L5 9 L4

=> d 15 ibib ab hitstr 1-9

L5 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2005:1042252 CAPLUS
DOCUMENT NUMBER: 143:326214
TITLE: Preparation of tricyclic benzopyran compounds as anti-arrhythmic agents
INVENTOR(S): Ohrai, Kazuhiko; Shigeta, Yukihiko; Uesugi, Osamu; Okada, Takumi; Matsuda, Tomoyuki
PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan
SOURCE: PCT Int. Appl., 445 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005090357	A1	20050929	WO 2005-JP6004	20050323
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: JP 2004-84605 A 20040323

AB Title compds. I [R1 and R2 independently = H, alkyl or aryl; R3 = H or alkylcarbonyloxy, or together with R4 forms a bond; R4 = H or together with R3 forms a bond, m is an integer of 0 to 4, n is an integer of 0 to 4, V = a single bond, substituted carbon linker, NH, O, etc.; R5 = H or alkyl; R6 = H, alkyl, cycloalkyl, cycloalkenyl, etc.; R7 and R8 or R8 and R9 together form a 5-, 6- or 7-member unsatd. ring fused with a benzene ring, as the constituent atoms of the ring there may be 1-3 O, N, or S atoms or a combination thereof, with the other R7 or R9 = H], or pharmaceutically acceptable salts thereof, are prepared and disclosed as antiarrhythmic agents. Thus, e.g., II was prepared via dehydrobromination of trans-3-bromo-2,2,7,9-tetramethyl-3,4-dihydro-2H-pyrano[2,3-g]quinolin-4-ol (preparation given) to form the intermediate epoxide which undergoes a regioselective ring opening reaction with 2-phenylethylamine. I selectively prolonged the effective refractory period of the atrium, e.g., II at 0.6 mg/kg prolonged the effective refractory period of the atrium by 21 ms. Pharmaceutical compns. are provided.

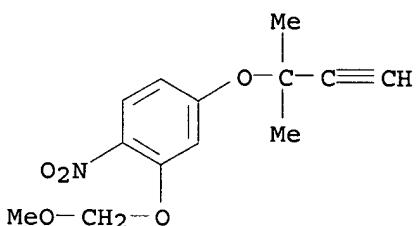
IT 865479-08-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of tricyclic benzopyran compound as anti-arrhythmic agents)

RN 865479-08-9 CAPLUS

CN Benzene, 4-[(1,1-dimethyl-2-propynyl)oxy]-2-(methoxymethoxy)-1-nitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:354900 CAPLUS
DOCUMENT NUMBER: 140:357051
TITLE: Process for production of an acetylenic compound
INVENTOR(S): Yamada, Osamu; Matsumoto, Hiroo; Shimizu, Takanori
PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan
SOURCE: PCT Int. Appl., 17 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

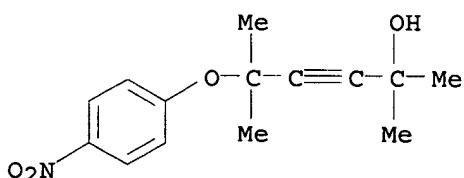
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004035520	A1	20040429	WO 2003-JP12312	20030926
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2502360	AA	20040429	CA 2003-2502360	20030926
EP 1564201	A1	20050817	EP 2003-748596	20030926
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
NO 2005002392	A	20050718	NO 2005-2392	20050518
JP 2002-303876 A 20021018				
WO 2003-JP12312 W 20030926				

PRIORITY APPLN. INFO.: OTHER SOURCE(S): CASREACT 140:357051

AB Disclosed is an industrial and economical process for producing an acetylenic compound (I), namely 1-[(1,1-dimethyl-2-propynyl)oxy]-4-nitrobenzene, from 4-nitrofluorobenzene, specifically, characterized by reacting 4-nitrofluorobenzene (II) with an alkoxide of 2-methyl-3-butyn-2-ol (III) at -20 to 10°. The acetylenic compound I is useful as an intermediate for drugs such as an antiarrythmic or antidepressant. Thus, 25.2 g III was added dropwise over 2 h to a suspension of 11.6 g 60% NaH (mineral oil suspension) and 96.0 g N,N-dimethylacetamide with ice-cooling and stirring, and stirred for another 30 min to give a solution of III sodium salt which was treated dropwise with 33.8 g 4-nitrofluorobenzene over 1.5 h under ice-cooling, stirred at the same temperature for 18 h, treated with 480 mL H2O and 480 mL p toluene, shaken to give, after workup and silica gel chromatog., 44.0 g I (90% yield).

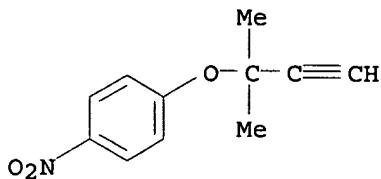
IT 682357-24-0P, 5-(4-Nitrophenoxy)-2,5-dimethyl-3-hexyn-2-ol
 RL: BYP (Byproduct); PREP (Preparation)
 (process for preparation of 1-[(1,1-dimethyl-2-propynyl)oxy]-4-nitrobenzene by etherification of 2-methyl-3-butyn-2-ol metal salt with 4-nitrofluorobenzene)

RN 682357-24-0 CAPLUS
 CN 3-Hexyn-2-ol, 2,5-dimethyl-5-(4-nitrophenoxy)- (9CI) (CA INDEX NAME)



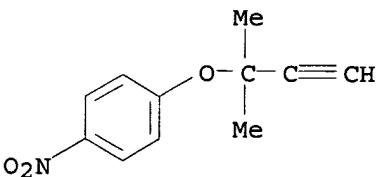
IT 2109-84-4P, 1-[(1,1-Dimethyl-2-propynyl)oxy]-4-nitrobenzene
 RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (process for preparation of 1-[(1,1-dimethyl-2-propynyl)oxy]-4-nitrobenzene by etherification of 2-methyl-3-butyn-2-ol metal salt with 4-nitrofluorobenzene)

RN 2109-84-4 CAPLUS
CN Benzene, 1-[(1,1-dimethyl-2-propynyl)oxy]-4-nitro- (9CI) (CA INDEX NAME)



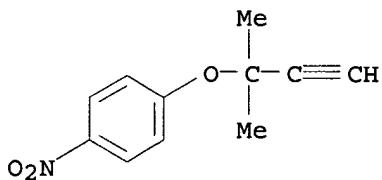
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:650939 CAPLUS
DOCUMENT NUMBER: 123:285380
TITLE: Copper(I) iodide: a catalyst for the improved synthesis of aryl propargyl ethers
AUTHOR(S): Bell, David; Davies, Mark R.; Geen, Graham R.; Mann, Inderjit S.
CORPORATE SOURCE: SmithKline Beecham Pharmaceuticals, Harlow, CM19 5AW, UK
SOURCE: Synthesis (1995), (6), 707-12
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Thieme
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:285380
AB Copper(I) iodide catalyzes the reaction between phenols $R_1C_6H_4OH$ ($R_1 = 4-O_2N$, 4-I, H, 3-CN, etc.) and dialkylpropargyl chlorides $HC.tpbond.CCR_2R_3Cl$ [$R_2 = R_3 = Me$, Et, $CHMe_2$; $R_2R_3 = (CH_2)_5$; $R_2 = Me$, $R_3 = Et$, CMe_3] to give aryl 1,1-dialkylpropargyl ethers, e.g. $PhOCMe_2C.tpbond.CH$, in good yields and purity. These ethers are important as precursors to the 2H-1-benzopyrans.
IT 2109-84-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of aryl propargyl ethers by copper(I) iodide-catalyzed reaction of phenols and dialkylpropargyl chlorides)
RN 2109-84-4 CAPLUS
CN Benzene, 1-[(1,1-dimethyl-2-propynyl)oxy]-4-nitro- (9CI) (CA INDEX NAME)



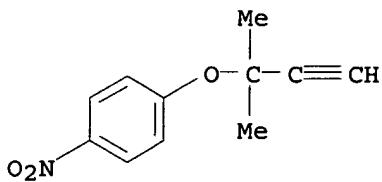
L5 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:65983 CAPLUS
DOCUMENT NUMBER: 122:9577
TITLE: Improved synthesis of aryl 1,1-dimethylpropargyl ethers
AUTHOR(S): Godfrey, Jollie D., Jr.; Mueller, Richard H.; Sedergran, Thomas C.; Soundararajan, Nachimuthu; Colandrea, Vincent J.

CORPORATE SOURCE: Chem. Process Research, Bristol-Myers Squibb,
 Princeton, NJ, 08543-4000, USA
 SOURCE: Tetrahedron Letters (1994), 35(35), 6405-8
 CODEN: TELEAY; ISSN: 0040-4039
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 122:9577
 AB An efficient, general, and practical synthesis of aryl 1,1-dimethylpropargyl ethers has been developed. Thus, alkylation of RC₆H₄OH (R = e.g., 4-CN, 4-NO₂) with HC₃CH₂Cl₂ (X = Cl, OCO₂Me, O₂CCF₃) in MeCN containing DBU and Cu salts resulted in high yield of propargyl ethers RC₆H₄OCMe₂CH₂CH=CH (up to 88%).
 IT 2109-84-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (synthesis of aryl 1,1-dimethylpropargyl ethers via copper-catalyzed alkylation of phenols with dimethylpropargyl chloride, carbonate, or trifluoroacetate)
 RN 2109-84-4 CAPLUS
 CN Benzene, 1-[(1,1-dimethyl-2-propynyl)oxy]-4-nitro- (9CI) (CA INDEX NAME)

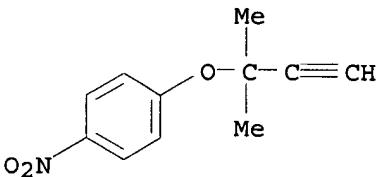


L5 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
 ACCESSION NUMBER: 1991:228481 CAPLUS
 DOCUMENT NUMBER: 114:228481
 TITLE: The synthesis and potassium channel blocking activity of some (4-methanesulfonamidophenoxy)propanolamines as potential class III antiarrhythmic agents
 AUTHOR(S): Connors, Sean P.; Dennis, Paul D.; Gill, Edward W.; Terrar, Derek A.
 CORPORATE SOURCE: Pharmacol. Dep., Oxford Univ., Oxford, OX1 3QT, UK
 SOURCE: Journal of Medicinal Chemistry (1991), 34(5), 1570-7
 CODEN: JMCMAR; ISSN: 0022-2623
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 114:228481
 AB The synthesis of 22 (4-methanesulfonamidophenoxy)propanolamines, e.g., I (R = Cl, CF₃, etc.) and their testing on isolated guinea pig cardiac myocytes, isolated preps. from guinea pig atria, and rat blood pressure are described. Secondary amines in the series showed residual β-blocking activity, whereas incorporation of N-Me phenylalkyl and 4-Ph alicyclic amine groups abolished β-blocking activity but led to enhanced ability to block the channel conducting the delayed rectified potassium current, and hence produced an increase in the cardiac action potential duration (APD). Incorporation of hydrophobic Cl and CF₃ groups further enhanced potassium channel blocking activity. I (R = Cl, CF₃) produced a significant increase in APD at nanomolar concns., with no effect on cardiac muscle conduction velocity, and hence merit further investigation as Class III antiarrhythmic agents. Methylation of the methanesulfonamido group abolished channel-blocking activity; 4-carboxy and 3-methanesulfonamido analogs retained activity but at a reduced level.
 IT 2109-84-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and cyclization of)

RN 2109-84-4 CAPLUS
CN Benzene, 1-[(1,1-dimethyl-2-propynyl)oxy]-4-nitro- (9CI) (CA INDEX NAME)



L5 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1990:178193 CAPLUS
DOCUMENT NUMBER: 112:178193
TITLE: A facile synthesis of aryl ethers of ethynyl-carbinols using the Mitsunobu reaction
AUTHOR(S): Subramanian, R. Sankara; Balasubramanian, K. K.
CORPORATE SOURCE: Dep. Chem., Indian Inst. Technol., Madras, 600 036, India
SOURCE: Synthetic Communications (1989), 19(7-8), 1255-9
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 112:178193
AB The synthesis of aryl ethers of ethynyl carbinols using the Mitsunobu reaction is reported. Thus, a mixture of HC.tplbond.CCMe2OH and 4-MeC6H4OH in C6H6 was treated with Ph3P and EtO2CN:NCO2Et to give 55% 4-MeC6H4OCMe2.tplbond.CH. Eleven similar examples are also reported.
IT 2109-84-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 2109-84-4 CAPLUS
CN Benzene, 1-[(1,1-dimethyl-2-propynyl)oxy]-4-nitro- (9CI) (CA INDEX NAME)



L5 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1977:535107 CAPLUS
DOCUMENT NUMBER: 87:135107
TITLE: Chroman derivatives
INVENTOR(S): Cata, John Morris Evans
PATENT ASSIGNEE(S): Beecham Group Ltd., UK
SOURCE: Ger. Offen., 20 pp.
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2702092	A1	19770728	DE 1977-2702092	19770119

GB 1548221	A	19790704	GB 1976-3024	19761217
FR 2339606	A1	19770826	FR 1977-1699	19770121
FR 2339606	B1	19810116		
AU 7721625	A1	19780803	AU 1977-21625	19770125
DK 7700319	A	19770728	DK 1977-319	19770126
SE 7700824	A	19770728	SE 1977-824	19770126
JP 52091866	A2	19770802	JP 1977-7613	19770126
NL 7700819	A	19770729	NL 1977-819	19770127

PRIORITY APPLN. INFO.:

GB 1976-3024	A 19760127
GB 1976-14239	A 19760408

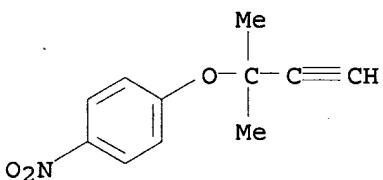
AB Piperidinobenzopyranyl esters I ($R = 6\text{-NO}_2$, $R1 = \text{Ac}$, Bz ; $R = 7\text{-NO}_2$, $R1 = \text{Ac}$) were prepared by esterification. I are antihypertensives. Thus, I ($R = 6\text{-NO}_2$, $R1 = \text{Bz}$) at 1 mg/kg orally in rats caused 26% decrease in blood pressure 1 h after administration.

IT 2109-84-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of)

RN 2109-84-4 CAPLUS

CN Benzene, 1-[(1,1-dimethyl-2-propynyl)oxy]-4-nitro- (9CI) (CA INDEX NAME)



L5 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1972:126142 CAPLUS

DOCUMENT NUMBER: 76:126142

TITLE: Influence of structure on the rate of thermal rearrangement of aryl propargyl ethers to the chromenes. Gem-dimethyl effect

AUTHOR(S): Harfenist, Morton; Thom, Edna

CORPORATE SOURCE: Burroughs Wellcome Co., Research Triangle Park, NC, USA

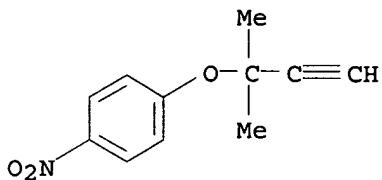
SOURCE: Journal of Organic Chemistry (1972), 37(6), 841-8
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The rates of first-order thermal cyclizations of a group of para-substituted aryl propargyl ethers $p\text{-ZC}_6\text{H}_4\text{OCRR}'\text{CH}$ (R , $R1 = \text{H}$ or Me) was determined in $\text{O}-\text{C}_2\text{H}_4\text{H}_4$ as a function of Z (OMe , NHAc , H , Cl , CN , NO_2) and of the number of Me groups. Where R and $R1$ are both H (k values extrapolated to 189.8°) or where R was Me and $R1$ was H (k values extrapolated to 161.6°), the points followed an adequate Hammett relation using σ^+ ($\rho = -0.43$) although the NO_2 and CN did not give a good fit for $R = R1 = \text{H}$, and $p\text{-Cl}$ was faster than $p\text{-H}$ for $R = \text{H}$, $R1 = \text{Me}$. The attempted Hammett plot for the gem-dimethyl analogs $R = R1 = \text{Me}$ had a paraboloid shape, e.g., $X = \text{NHAc}$ and $X = \text{NO}_2$ had about the same rate, with $X = \text{H}$ at a min. (k values extrapolated to 161.6°). The $\Delta S_{\text{++}}$ and $\Delta H_{\text{++}}$ followed no obvious order. The results are best explained by assuming that the gem-dimethyl effect results from an increase in the proportion of the rotamer with the ethynyl group positioned near the benzene ring, i.e., the rotamer best positioned for reaction, when no H is available to rotate to that position, and that activation of the position meta to the substituent Z , at least by the electron-withdrawing groups, exists. Preparative runs showed that an essentially quant. yield of 2-methyl or 2,2-dimethyl-3-chromenes could be obtained.

IT 2109-84-4P
 RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
 (preparation and kinetics of cyclization of)
 RN 2109-84-4 CAPLUS
 CN Benzene, 1-[(1,1-dimethyl-2-propynyl)oxy]-4-nitro- (9CI) (CA INDEX NAME)



L5 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1965:438866 CAPLUS
 DOCUMENT NUMBER: 63:38866
 ORIGINAL REFERENCE NO.: 63:6917g-h,6918a-b
 TITLE: p-tert.-Alkoxyanilines
 PATENT ASSIGNEE(S): Wellcome Foundation Ltd.
 SOURCE: 20 pp.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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NL 6406078		19641201	NL	
PRIORITY APPLN. INFO.:			GB	19630531
AB	p-RR ₁ R ₂ COC ₆ H ₄ NR ₃ COR ₄ (I) is prepared by treating p-O ₂ NC ₆ H ₄ F with KOCRR ₁ R ₂ to give p-O ₂ NC ₆ H ₄ OCRR ₁ R ₂ (II), reduction of II to H ₂ NC ₆ H ₄ OCRR ₁ R ₂ (III), then preparation of p-RR ₁ R ₂ COC ₆ H ₄ NHCOR ₄ (IV) by adding R ₄ COX to III, and reduction of			
of	IV, followed by reaction with R ₄ COX. Thus, 254 g. p-O ₂ NC ₆ H ₄ F was added to 200 g. KOCMe ₃ in 1200 ml. HOCMe ₃ and the mixture heated at 100° for 15 min., giving II (R = R ₁ = R ₂ = Me) (V), b0.4 112-14°. V(39 g.) in 200 ml. EtOH and 12 g. AcOH was hydrogenated with H (Pt catalyst) to give the corresponding amine, which with 25 g. Ac ₂ O gave IV (R = R ₁ = R ₂ = R ₄ = Me), m. 131-2°. Reduction with Li-AlH ₄ and reaction with Ac ₂ O gave I (R = R ₁ = R ₂ = R ₄ = Me, R ₃ = Et), m. 50-3°. Similarly prepared were the following I (R, R ₁ , R ₂ , R ₃ , R ₄ , and m.p. given): Me, Me, Me, H, H, 74°; Me, Me, Me, H, Et, 101°; Me, Me, Me, H, Pr, 126-30°; Me, Me, Me, Me, 80-1°; Me, Me, Me, Pr, Me, - (b0.01 133°); Me, Me, Et, H, Me, 113° (corresponding II b0.03 93-102°); Me, Me, (Me ₂ C(OH)CH ₂ CH ₂ , H, Me, 106-8° (corresponding II b0.2 166-8°); Et, Et, Me, H, Me, 102.6-104° (corresponding II b0.015 98-105°); Me, Me, HC:C, H, Me, 83-4° (corresponding II b0.01 96-100°). These compds. can be used as sedatives and as stimulants.			
IT	2109-84-4, Ether, 1,1-dimethyl-2-propynyl p-nitrophenyl (preparation of)			
RN	2109-84-4 CAPLUS			
CN	Benzene, 1-[(1,1-dimethyl-2-propynyl)oxy]-4-nitro- (9CI) (CA INDEX NAME)			

